Abrupt-Kink Model of Dislocation Motion. II

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The abrupt-kink model of dislocation motion is generalized to describe the dynamics of a dislocation at temperatures where the barrier to kink diffusion is negligible compared with the thermal energy, and where generation of double kinks is still unimportant. It is assumed that kinks may be treated as a one-dimensional gas of particles which interact through their long-range stress fields. The interaction energy, $U(x)$, at a separation x is derived. For x greater than a few lattice spacings, $U(x)\sim|x|^{-1}$, like the interaction between point charges. The equations of motion of a dislocation are obtained for a general $U(x)$. It is shown that the well-known string model is equivalent to assuming an incorrect short-range interaction $U(x)\sim\delta(x)$ and ignoring the variation of the effective mass of a dislocation with its orientation relative to a close-packed crystal direction. While the equations of motion have not been solved with the true interaction, possible effects of its long-range character are investigated with an interaction of the form $U(x)\sim-\ln|x|$. The behavior of the dislocation under a static stress is discussed according to this model and, in addition, the fundamental frequency of vibration about the equilibrium configuration is derived.

I. INTRODUCTION

In a previous paper[1] (subsequently referred to as I), a new model of dislocation motion was presented. The essential feature of this model was the recognition given to the discrete atomic nature of a dislocation through introduction of the concept of an abrupt kink. Further, it was shown how macroscopic equations of motion of a dislocation could be obtained from the microscopic properties of an abrupt kink.

We were concerned in I with the temperature regime in which the mean thermal energy of a kink was less than the activation energy for kink diffusion. A first application of the theory to internal friction phenomena was shown to account for many of the finer details of the Bordoni attenuation peak which is found experimentally in cold worked metals.

According to our interpretation of the origin of the Bordoni peak, the activation energy for kink diffusion in fcc metals would appear to be ~0.08 eV. While *a priori* this value seems quite reasonable to us, in view of the present lack of definite confirmatory experimental evidence for our interpretation, one cannot yet exclude the possibility that some other mechanism is operative in producing the observed attenuation. Thus, in the interim, we have been considering an alternative formulation of the abrupt kink model which would be applicable if the mean thermal energy of a kink were considerably larger than the activation energy for kink diffusion. Of course, if our previous estimate of the activation energy is correct, the contents of this paper are totally irrelevant for fcc metals, since the metal would then no longer be a solid. But, in any event, it is conceivable that the activation energy can vary significantly from one structure to another among the different types of solids. Consequently, at this early stage, it seems worthwhile to explore other possible formulations of the model if only to determine the qualitative behavior of a dislocation under the differing conditions which may be hypothesized. However, we should emphasize that the present treatment is in no way meant to compromise the model as outlined in I. Rather, it is our hope that the pertinent conditions for any particular solid can be resolved by further experimental study.

As in I, we shall continue to assume that the thermal generation of double kinks may be neglected at temperatures of interest. Consequently, the motion of a dislocation will be described again in terms of the behavior of those kinks which are "built-in" at 0°K by virtue of its orientation relative to a particular close-packed direction.

The application of an external stress tends to drive kinks of the same type toward one pinning point. Thus, in order to obtain a finite compliance, the model must include some mechanism which opposes such a redistribution of kinks. In I this was attributed to the diffusive character of the kink motion. Thereby the tendency to avoid a large concentration gradient of kinks was explicitly included. However, if the barrier height for kink diffusion is negligible, such a mechanism is inoperative. Obviously, in this instance, the behavior of a dislocation must be governed largely by the long-range interaction between the different kinks of which it is constituted. The origin of this interaction is clearly through the elastic stress field associated with a kink.

In the next section, we shall consider the following model. It will be assumed that the concept of the kinetic energy of a kink is valid. With this premise, the problem of determining the collective behavior of a set of kinks or of a one-dimensional gas become formally identical. The latter can be formulated in terms of elementary hydrodynamics. In the present context, a similar treatment yields (after minor approximation), and for an arbitrary kink-kink interaction, the equation of motion of the dislocation. The latter is an integro-differential equation in which the kernel is the kink-kink interaction energy, $U(x)$. Thereby, it manifests specifically the manner in which the motion of a particular line element is influenced by the configuration of the remainder of the dislocation. Moreover, the circumstance in which an analogy with an extensible string

[1] A. D. Brailsford, Phys. Rev. 122, 778 (1961).

might exist is immediately obvious. For since the motion of a line segment of a string depends only upon the configuration at the same point, it is easily shown that $U(x)$ would have to assume a δ-function character.

The correct form of $U(x)$ is therefore of some potential interest. It is derived, following a method due to Burgers, in Sec. III. We find that, at large distances, $U(x)\sim|x|^{-1}$, a behavior typical of the interaction between point charges. Thus, in contrast to the requirement for a string model, the interaction is of long range.

Unfortunately, the structure of $U(x)$ does not appear to lend itself readily to analysis in the one-dimensional problem under consideration. However, since the essential feature is its long-range character, it is interesting to investigate a further hypothetical example which does incorporate this property, so that one may anticipate some consequences of the correct interaction. Accordingly, in Sec. IV, we consider the behavior of a dislocation for a supposed interaction $U(x)\sim-\ln|x|$. This example has two virtues. First, the whole analysis is trivial. And, secondly, it may be of incidental interest to any reader concerned with the separate problem of the dynamical properties of a pile-up of rigid dislocations. For the present work, the most interesting prediction appears to be the form of the equilibrium configuration of a dislocation. Namely that, instead of lying straight along the line joining the two pinning points, a dislocation with built-in kinks possesses macroscopic curvature even in the absence of an applied stress.

The preceding description outlines the contents of this paper. Inasmuch as we consider here that kinks are free to move along a dislocation, the model bears some superficial resemblance to other work in dislocation theory involving kinks. As a consequence of this apparent similarity, it is possible that certain remarks we have made could be the source of confusion unless we explain further our particular point of view. In particular, we refer to the discussion of the analogy with an extensible string. In the past it has been proposed that the form of a kink in a dislocation could be *derived* from the model of a string with line tension subject, in addition, to a spatially periodic force field which in some manner is meant to account for the structure of the host lattice.[2] Thus, from this standpoint a dislocation could never behave like an extensible string alone. But the question is, can one really separate the totality of all the atomic forces, as implied by this model, in such a way meaningly? Indeed, it may be possible. But, unfortunately, we do not know how to do it. Instead we prefer to adopt the following hypothesis. Namely, kinks exist, *ipso facto*. That is,[3] "A kink is to a dislocation what a dislocation is to a slip plane." It represents a fundamental unit of atomic dimensions. Then, with additional assumptions concerning the character of the kink motion, we show here, as in I, how a macroscopic description of the static or dynamic properties of a dislocation may be derived. In our opinion, it is only in this latter description that comparison with models derived from a continuum theory are justified.

[2] A. Seeger, Phil. Mag. **1**, 651 (1956).
[3] A. W. Overhauser (private communication).

II. EQUATION OF MOTION

In order to be specific, we shall discuss the behavior of a dislocation which is inclined, on the average, at an angle θ to a close-packed direction and contains a sequence of built-in "left" kinks. The notation (and vocabulary) follow that used in I. An (x,y) coordinate system is chosen in which the x axis is parallel to a close-packed direction, the two pinning points being located at $(-L/2,0)$ and $(L/2,L\tan\theta)$. Thus, we wish to determine the kink density $n(x,t)$, under the new conditions we have postulated. The position of the dislocation, $y(x,t)$, can then be obtained by simple integration:

$$y(x,t)=a\int_{-L/2}^{x}n(x,t)dx. \tag{1}$$

As a first approximation we shall assume that the interaction between kinks depends only upon the variable x and is independent of their relative orientation with respect to the close-packed direction. Of course, this is incorrect in detail (see Sec. III), but the error involved is generally small. As a result, one can achieve considerable mathematical simplification without compromising the physical features in any essential way. The problem is then one-dimensional.

According to the basic tenets of the model, for a given interaction, the equation of motion of a kink may be obtained from Newton's Law. However, our basic objective is better served by treating the kink assembly as a one-dimensional fluid. For we are not so much interested in the motion of any individual kink as in the time development of the macroscopic density. Thus, if we introduce a drift velocity $v(x,t)$, the equations of motion may be written in the form:

$$\partial n/\partial t+(\partial/\partial x)(nv)=0, \tag{2}$$

and

$$\partial v/\partial t+(\partial/\partial x)(v^2/2)=F(x)/m_k. \tag{3}$$

Here, m_k is the effective mass of a kink and $F(x)$ is the total force acting on a kink at x, which, in the presence of a constant applied stress σ, is

$$F(x)=-\int_{-L/2}^{L/2}n(x')\frac{\partial U(x-x')}{\partial x}dx'-\sigma ab. \tag{4}$$

Equations (2) and (3) are, respectively, the equation of continuity and Euler's equation. They may be derived either by standard methods or, formally, from the Lagrangian of the many-particle (kink) assembly. For general interest, the latter derivation is presented in the Appendix.

The equations of motion have to be supplemented by appropriate boundary conditions. We assume that the dislocation is firmly pinned at $x=\pm L/2$. The boundary conditions are therefore

$$v=0, \quad \text{at} \quad x=\pm L/2. \tag{5}$$

In addition, there is the further constraint

$$\int_{-L/2}^{L/2} n(x)dx=n_0L, \tag{6}$$

where n_0 is the average kink density, which defines the relative orientation of the pinning points in the slip plane.

When departures from the equilibrium distribution, $n_e(x)$, are small, the equation determining the kink density can be obtained readily from (2) and (3). For, if we let

$$n(x,t)=n_e(x)+n_1(x,t), \tag{7}$$

where $n_e(x)$ satisfies the integral equation

$$\int_{-L/2}^{L/2} n_e(x')\frac{\partial U(x-x')}{\partial x}dx'+\sigma ab=0, \tag{8}$$

we obtain, to first order, the following equation for n_1:

$$\frac{\partial^2 n_1(x,t)}{\partial t^2}=\frac{1}{m_k}\frac{\partial}{\partial x}\left\{n_e(x)\frac{\partial}{\partial x}\int_{-L/2}^{L/2} n_1(x',t)U(x-x')dx'\right\}. \tag{9}$$

Or, by virtue of (1), after integration,

$$\frac{\partial^2 y_1(x,t)}{\partial t^2}=\frac{1}{m_k a}\left\{\frac{\partial y_e(x)}{\partial x}\right\}\frac{\partial}{\partial x}\int_{-L/2}^{L/2}\frac{\partial y_1(x',t)}{\partial x'}U(x-x')dx'. \tag{10}$$

This constitutes the equation of motion of a dislocation according to the present formulation of the abrupt-kink model. Through its integral character it illustrates explicitly that the displacement at one point is affected by the configuration of the remainder of the dislocation.

Although (10) is quite complicated in structure, it is not difficult to determine the approximation in which the equation describes the motion of a flexible string. For as we have stated in the previous section, the equation must then be of completely local character. This suggests that we examine the consequence of an interaction of the type

$$U(x)=Sa^2\delta(x-x'), \tag{11}$$

where S is constant. And, indeed, for $\sigma=0$, we find from (8) that (10) reduces to

$$\frac{\partial^2 y_1}{\partial t^2}=\frac{Sn_0a^2}{m_k}\frac{\partial^2 y_1}{\partial x^2}, \tag{12}$$

which is the equation determining the displacement of a flexible string with line tension S. However, there is still one important difference from the model which is normally used,[4] namely, that the effective mass per unit length m^*, is here given by

$$m^*=m_k/n_0a^2. \tag{13}$$

Thus, if one assumes an effective mass for a kink, the effective mass of unit length of a dislocation depends upon the average kink density. This is an obvious physical consequence of the fundamental mechanism of the dislocation motion.

We have shown that an interaction if the type (11) yields a modified version of the string model. Clearly it is of interest to establish the true nature of $U(x)$. This will be the object of the following section.

III. INTERACTION BETWEEN KINKS

As an example, we consider the dislocation shown in Fig. 1(a). The Burgers vector **b** is at an angle Φ to the close-packed direction, the slipped region in the slip plane being labeled S. The burden of this section will be to determine the effective force on the kink A arising from the presence of the other kinks in the dislocation.

The method is based upon the following observation: Namely, that the dislocation in 1(a) can be represented as a superposition of a dislocation $0AB$, with one kink, and of a sequence of two-cornered dislocations as shown in Fig. 1(b). If, by convention, we call the dislocation $0AB$ positive, these two cornered dislocations will be positive or negative also, depending upon whether they lie to the right or left, respectively, of A. Let σ_D represent the component of the shear stress acting in the slip plane, in the slip direction, at A, due to dislocation with corners near D. Then the effective force f_{AD},

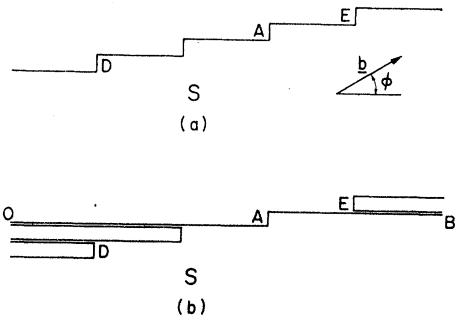

FIG. 1. (a) A dislocation containing a sequence of left kinks and (b) an equivalent dislocation network.

[4] A. Granato and K. Lucke, J. Appl. Phys. **27**, 583 (1956).

exerted by the kink at D upon that at A is

$$f_{AD}=-\sigma_D ba. \tag{14}$$

The calculation of σ_D will be presented below.

The displacement field resulting from a two-cornered dislocation of the above type can be obtained from the general result of Burgers.[5] Following his notation, with the coordinate system given in Fig. 2, we find the displacement, $\mathbf{u}(\mathbf{r})$, to be

$$\mathbf{u}(\mathbf{r})=\mathbf{u}^*(\mathbf{r})+\mathbf{u}^{**}(\mathbf{r})+\text{grad}\psi, \tag{15}$$

where

$$\mathbf{u}^*(\mathbf{r})=\frac{\mathbf{b}}{4\pi}\Big[\tan^{-1}\Big(\frac{y+a}{z}\Big)-\tan^{-1}\Big(\frac{y}{z}\Big)+\tan^{-1}\Big(\frac{xy}{zr}\Big)-\tan^{-1}\Big(\frac{x(y+a)}{zr_q}\Big)\Big], \tag{16}$$

$$u_x^{**}(\mathbf{r})=u_y^{**}(\mathbf{r})=0, \tag{17}$$

$$u_z^{**}(\mathbf{r})=\frac{b}{4\pi}g(\mathbf{r},\Phi), \tag{18}$$

$$\psi(\mathbf{r})=\frac{-bz}{8\pi(1-\nu)}g(\mathbf{r},\Phi), \tag{19}$$

and

$$g(\mathbf{r},\Phi)=(\sin\Phi)\ln\Big(\frac{r+x}{r_q+x}\Big)+(\cos\Phi)\ln\Big(\frac{r+y}{r_q+y+a}\Big). \tag{20}$$

In these equations, ν is Poisson's ratio and r_q is the distance of $\mathbf{r}$ from the point Q, i.e.

$$r_q=[x^2+(y+a)^2+z^2]^{1/2}. \tag{21}$$

These displacements can be used to compute the stress σ_D and hence the force f_{AD}. After some algebra, one can show that f_{AD} may be written in the following form

$$f_{AD}=-(\partial/\partial x)U(\varrho,\Phi), \tag{22}$$

which defines the kink-kink interaction energy, U. We find that

$$U(\varrho,\Phi)=\frac{\mu ab^2}{4\pi(1-\nu)}\Big\{(1-\nu\cos^2\Phi)\Big[\Big(\frac{\rho-x}{y}\Big)-\Big(\frac{\rho_q-x}{y+a}\Big)\Big]+(1-\nu\sin^2\Phi)\ln\Big(\frac{\rho_q+y+a}{\rho+y}\Big)+(\nu\sin2\Phi)\ln\Big(\frac{\rho_q+x}{\rho+x}\Big)\Big\}, \tag{23}$$

where

$$\rho=(x^2+y^2)^{1/2},\quad \rho_q=[x^2+(y+a)^2]^{1/2}, \tag{24}$$

and μ is the shear modulus. Since we can expect (23) to be correct only for separations much larger than a lattice constant, we expand U as a power series in the kink height, a. We then obtain the comparatively simple result

$$U(\varrho,\Phi)\simeq\frac{\mu a^2b^2}{8\pi(1-\nu)}\frac{1}{\rho}\{(1+\nu-3\nu\sin^2\Phi)+t[(1-\nu\cos^2\Phi)t+2\nu\sin2\Phi]\}, \tag{25}$$

where $t=\tan(\theta/2)$, and $\tan\theta=(y/x)$. Evidently, the interaction between like kinks is repulsive and varies inversely as their separation. In a similar manner, one can see that the interaction between unlike kinks would be of the same form as (25) but with opposite sign (i.e., attractive). For the only change in the analysis would be a change of sign in (14). Moreover, it is easy to show that kinks (such as E) to the right of A obey the same interaction law.

Finally, we would point out that for $\theta\lesssim\pi/4$, U does not depend in any essential way upon the relative orientation of the two kinks with respect to a close-packed direction. Thus, as we mentioned in the previous section, a further reasonable approximation to U is

$$U(x)\simeq\frac{\mu a^2b^2}{8\pi(1-\nu)}\frac{1}{|x|}(1+\nu-3\nu\sin^2\Phi),\quad (|x|\gg a) \tag{26}$$

for kinks of the same type.

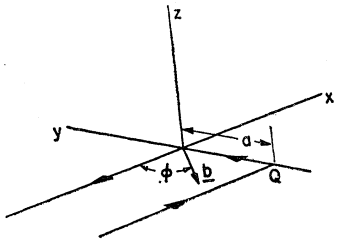

FIG. 2. The coordinate system used in calculating the stress field arising from a two-cornered dislocation.

IV. EFFECT OF LONG-RANGE INTERACTION

Although $U(x)$ has the simple asymptotic form given above, we have not yet been able to devise an analytic method of solution of the equation of motion with this interaction. While we could have resorted to numerical analysis, it appeared more worthwhile at this point to seek an alternative hypothetical interaction which, although making the problem easily soluble, would contain the essential long-range character of the correct interaction. Thus, we were led to consider the consequences of an interaction

$$U(x)=-U_0\ln|x|, \tag{27}$$

U_0 being constant. Of course, (27) tends to overestimate the long-range effects. But in view of the stated aim of the exercise, this does not cause any special concern.

We will consider first the steady-state configuration in the presence of an applied stress. Substituting for

[5] J. M. Burgers, Proc. Acad. Sci. Amsterdam 42, 293 (1939).

$U(x)$, Eq. (8) becomes

$$\int_{-L/2}^{L/2} \frac{n_e(x')}{(x-x')}dx' - \left(\frac{\sigma ab}{U_0}\right) = 0. \tag{28}$$

This equation can be solved by the following method. We let $x = (L/2)\cos\Phi$ and use the expansion

$$\frac{1}{\cos\Phi - \cos\Phi'} = -2\sum_{n=1}^{\infty} \frac{\sin(n\Phi)}{\sin\Phi} \cos n\Phi'. \tag{29}$$

Hence, if $n_e(x) = P(\Phi)$, (28) becomes

$$\sum_{n=1}^{\infty} \sin n\Phi \int_0^{\pi} P(\Phi') \sin\Phi' \cos n\Phi' d\Phi' = -(\sigma ab/2U_0)\sin\Phi, \tag{30}$$

or

$$\int_0^{\pi} P(\Phi') \sin\Phi' \cos n\Phi' d\Phi' = -\delta_{n,1}(\sigma ab/2U_0). \tag{31}$$

The solution of (31) is

$$P(\Phi)\sin\Phi = K - (\sigma ab/\pi U_0)\cos\Phi, \tag{32}$$

where K is a constant, to be determined from (6). Thus, in terms of the original variables, one finds the position of the dislocation to be given by

$$y = (n_0 aL/\pi)[\pi - \cos^{-1}(2x/L)] + (\sigma a^2 bL/2\pi U_0)[1-(2x/L)^2]^{1/2}. \tag{33}$$

This is an interesting result. It shows that, even in the absence of an external stress, the dislocation is not straight. As a result of the long-range interaction, kinks tend to pile up near the pinning points, producing thereby a macroscopic curvature in the dislocation.

In addition, we should note the condition in which (32) is a physically allowable solution. Since the generation of double kinks is prohibited, it is clear that, in our example, $(dy/dx) \geq 0$. That is, the density $n(x)$ must be everywhere positive. Since $K = (2n_0/\pi)$, it is evident from (32) that the solution is valid only for stresses less than a critical stress, σ_c, given by

$$\sigma_c = 2n_0 U_0/ab. \tag{34}$$

For larger stresses, and near the pinning point at $(L/2, L\tan\theta)$, the dislocation is constrained to lie along the close-packed direction.

Finally, we shall derive the fundamental frequency of vibration of the dislocation with the model interaction (27). We consider only the simplest situation when there is no applied stress. Then substitution into (10), with the same change of variable as given above, yields the equation

$$-\omega^2 Y(\Phi)\sin\Phi = \frac{4n_0 U_0}{\pi L m_k}\int_0^{\pi} \frac{\partial Y(\Phi')/\partial\Phi'}{(\cos\Phi - \cos\Phi')}d\Phi', \tag{35}$$

where $y_1 = Y(\Phi)$ and we have assumed a time dependence $y_1 \sim \exp(i\omega t)$. Since y_1 must be zero at the pinning points, we make the expansion

$$Y(\Phi) = \sum_{n=1}^{\infty} A_n \sin n\Phi. \tag{36}$$

Then, by virtue of (29), we obtain

$$\omega^2 \sin^2\Phi \sum_{n=1}^{\infty} A_n \sin n\Phi = \omega_0^2 \sum_{n=1}^{\infty} nA_n \sin n\Phi, \tag{37}$$

where

$$\omega_0^2 = (4n_0 U_0/Lm_k). \tag{38}$$

Hence, the A_n satisfy the relations

$$A_1(3-2\gamma) = A_3, \tag{39}$$

and, for $n \geq 2$

$$A_{n+2} = 2(1-\gamma n)A_n - A_{n-2}, \tag{40}$$

where $A_0 = 0$, and $\gamma = (2\omega_0^2/\omega^2)$. Three-term recurrence relations of the general type (40) occur also in solutions of Mathieu's equation.[6] Only for certain values of γ, with fixed A_1 and A_2, will the sequence of numbers A_n converge. These values of γ correspond to the normal vibrational frequencies. The fundamental frequency can be found readily using the techniques employed for solving Mathieu's equation. Thus, with $A_n \equiv 0$ for all odd n, we find $\omega \approx 1.8\omega_0$, whereas for $A_n \equiv 0$ for all even n, we obtain $\omega \approx 1.1\omega_0$. Hence, the fundamental frequency, ω_f, is $\omega_f \approx 1.1\omega_0$. Although the numerical coefficient is of no practical interest, the form of ω_0 illustrates again the dependence of the vibrational frequency upon the orientation relative to a close-packed direction and the strength of the kink-kink interaction.

V. SUMMARY AND CONCLUSION

The abrupt-kink model of dislocation motion has been reformulated so as to include the temperature regime in which the mean thermal energy of a kink is much greater than the activation energy for kink diffusion. The equation of motion of a dislocation has been derived for an arbitrary kink-kink interaction. The form of this interaction has been obtained. While we have not been able to solve the equation of motion with the correct interaction, a model incorporating its long-range property has been investigated in detail.

It should be obvious from the treatments given here and in I that any of the presently conceived aspects of dislocation motion can be described within the framework of the abrupt-kink model. But since, for a particular temperature, the conditions covered by the two formulations are mutually exclusive, the definitive determination of the activation energy for kink diffusion

[6] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), p. 556.

in dislocations of different types is obviously of paramount interest. It is our hope that this can be established by further experimental and theoretical study.

ACKNOWLEDGMENT

I wish to thank Dr. A. W. Overhauser for his continued interest in this work.

APPENDIX

The Lagrangian, L, of a set of kinks at positions, x_i, is

$$L=\tfrac{1}{2}m_k\sum_i \dot{x}_i^2-\tfrac{1}{2}\sum_{i,j,(i\neq j)} U(|x_i-x_j|). \quad \text{(A1)}$$

We wish to determine the time development of the macroscopic density, $n(x)$. Since

$$n(x)=\textstyle\sum_i \delta(x-x_i), \quad \text{(A2)}$$

apart from self-energy terms, which we can ignore, the total potential energy, V, may also be rewritten as

$$V=\frac{1}{2}\int_{-L/2}^{L/2}dx\int_{-L/2}^{L/2}dx'\ U(|x-x'|)n(x)n(x'). \quad \text{(A3)}$$

Our aim will be to express the kinetic energy in terms of similar collective variables, and hence derive the equations of motion.

We introduce the complex Fourier transform, n_q, by means of the relation

$$n_q=L^{-1/2}\int_{-L/2}^{L/2}n(x)e^{-iqx}dx. \quad \text{(A4)}$$

That is, from (A2),

$$n_q=L^{-1/2}\textstyle\sum_i e^{-iqx_i}. \quad \text{(A5)}$$

Then, the momentum, Φ_{-q} say, canonically conjugate to n_q is given by

$$\Phi_{-q}=\partial L/\partial\dot{n}_q. \quad \text{(A6)}$$

But since

$$p_i=\frac{\partial L}{\partial\dot{x}_i}=\sum_q \Phi_{-q}\frac{\partial\dot{n}_q}{\partial\dot{x}_i}, \quad \text{(A7)}$$

we find, after differentiating (A5) with respect to time, that

$$p_i=-iL^{-1/2}\sum_q \Phi_{-q}qe^{-iqx_i}. \quad \text{(A8)}$$

Hence, the kinetic energy, T, of the system is

$$T=\sum_i (p_i^2/2m_k)$$

$$=(1/2m_kL^{1/2})\sum_{q,q'} qq'\Phi_{-q}\Phi_{q'}n_{q-q'}, \quad \text{(A9)}$$

or

$$T=(1/2m_k)\int_{-L/2}^{L/2}n(x)(\partial\Phi/\partial x)^2dx, \quad \text{(A10)}$$

where

$$\Phi_q=L^{-1/2}\int_{-L/2}^{L/2}\Phi(x)e^{-iqx}dx. \quad \text{(A11)}$$

Equation (A10) will be recognized as the kinetic energy of a fluid when expressed in terms of a velocity potential $\Phi(x)/m_k$. The equations of motion for n and Φ may be found from the Hamiltonian, $H=T+V$. After the substitution $m_kv(x)=\partial\Phi/\partial x$, the latter yield Eqs. (2) and (3) of the text.

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Nuclear Magnetic Resonance in UAl_2

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The nuclear magnetic resonance of Al^{27} in UAl_2 has been observed in the range of temperatures 4–300°K. Large Knight shifts (K) were found with a temperature dependence not of a Curie-Weiss type. This behavior and the temperature independence of the linewidth, when considered in conjunction with susceptibility (χ) measurements, indicate (1) no localization of the magnetization of the U (5f and/or 6d) electrons and (2) no magnetic ordering exists. These results are contrasted with those obtained on the isostructural XAl_2 (X=rare-earth ion) metals. Using a simple model, certain features of the band structure and the effective exchange interaction between itinerant f and s electrons may be deduced. From the extrapolated limit of the linear K vs χ curve a large positive temperature-independent contribution to χ is obtained which is attributable to the Kubo-Obata orbital paramagnetism to be expected in metals with unfilled degenerate bands.

INTRODUCTION

EXPERIMENTAL evidence of an appreciable exchange interaction between the localized spin moments of the rare-earth ions and the conduction electrons has been obtained from nuclear magnetic resonance (NMR) studies[1] of the XAl_2 intermetallic

[1] V. Jaccarino, B. T. Matthias, M. Peter, H. Suhl, and J. H. Wernick, Phys. Rev. Letters 5, 251 (1960).